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CRITICAL PERCOLATION STRESSES OF RANDOM FRANK-READ SOURCES IN MICRON-SIZED CRYSTALS OF SUPERALLOYS (Preprint)

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14. ABSTRACT
Effective 2D dislocation dynamics simulations were used to investigate the size effect observed experimentally in the yield behavior of micron-sized crystals of 2-phase superalloys. Random Frank-Read sources were introduced on a (111) glide plane for three simulation cell sizes. The critical stresses were determined for the percolation of Frank-Read sources in such cells populated with a distribution of γ' precipitates at ~ 73.5% vol fraction obtained from experiment. The scatter in the percolation stress at each size, as well as the weak variation in critical stress with size, were compared with experimental 0.2% yield stress values for micron-sized crystals of superalloy and found to be in good agreement. An APB energy of 250 mJ/m2 was used in the simulations. The size effect and scatter were found to be related to two factors: 1) Strength of single-arm sources as well as 2) the variation in precipitate structure at the single arm source positions.

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Critical Percolation Stresses of Random Frank-Read Sources in Micron-Sized Crystals of Superalloys

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Abstract

Effective 2D dislocation dynamics simulations were used to investigate the size effect observed experimentally in the yield behavior of micron-sized crystals of 2-phase superalloys. Random Frank-Read sources were introduced on a (111) glide plane for three simulation cell sizes. The critical stresses were determined for the percolation of Frank-Read sources in such cells populated with a distribution of γ' precipitates at ~ 73.5% vol fraction obtained from experiment. The scatter in the percolation stress at each size, as well as the weak variation in critical stress with size, were compared with experimental 0.2% yield stress values for micron-sized crystals of superalloy and found to be in good agreement. An APB energy of 250 mJ/m^2 was used in the simulations. The size effect and scatter were found to be related to two factors: 1) Strength of single-arm sources as well as 2) the variation in precipitate structure at the single arm source positions.

Keywords: superalloys; dislocation dynamics, size effect; yield stress; precipitation hardening

Experimental studies have shown that micrometer-scale face-centered cubic crystals show strong strengthening effects, even at high initial dislocation densities [1-3]. Similar behavior has been observed for microcrystals of two-phase superalloys [4]. Previously, large-scale 3-D discrete dislocation simulations (DDS) were used to explicitly model the pure compression deformation behavior of FCC materials under single-slip conditions [5-8]. The simulation study showed that two size-sensitive athermal hardening processes, beyond forest hardening, are *sufficient* to develop the dimensional scaling of the flow stress, stochastic stress variation, flow intermittency and, high initial strain-hardening rates, similar to experimental observations for various FCC materials [5,9]. One mechanism, source-truncation hardening, is especially potent in micrometer-scale volumes [5]. A second mechanism, termed exhaustion hardening, occurs because of deviations from mean-field conditions for forest hardening in small volumes, thus biasing the statistics of ordinary dislocation processes [5, 10-12].

In this study, 2D dislocation dynamics simulations of the percolation of a<110> superdislocation Frank-Read sources through an experimentally determined γ' precipitate distribution in micron-sized superalloys, are used to examine whether the source-truncation mechanism explains the initial yield behavior of these superalloys. The experimental quantities considered were the level of initial yield stress as a function of size as well as the scatter in the yield stress at each size [4]. Only, the APB interaction was considered for the precipitate-dislocation interaction, with an APB energy of 250 mJ/m^2 [13]. We used the 3D massively parallel dislocation dynamics code, ParaDiS [14], modified for the precipitate-dislocation APB interaction, to carry out these simulations.

Superdislocation Frank-Read sources, having random positions, sizes and orientations, were introduced on a {111} glide plane of simulation cells having three different sizes, 2.75 X 4.125 micron, 5.5 X 8.25 micron and 11 X 16.5 micron. The superdislocation was divided into two a/2<110> superpartials and each superpartial was divided into linear segments having a maximum size of 5a<110>. The two superpartials were separated by 2 nm in the initial configuration. The Frank-Read source pinning points were constrained to lie in the matrix. Free surface boundary conditions were applied in the simulations [5]. The {111} glide planes were populated with an experimentally determined size and spatial precipitate distribution, obtained from a Scanning Electron Microscope (SEM) micrograph (see Figure 1). The volume fraction of γ' precipitates in this superalloy was 73.5%. The precipitate distribution was voxellized into 2.75 X 2.75 nm cells, with the cells digitized to a value of 0 or 1, 0 – no precipitate within the voxel, 1 – precipitate within the voxel. If a dislocation node belonging to the leading superpartial lies inside a voxel with a precipitate, the precipitate exerts a retarding force of γ per unit length on the dislocation, where γ is the APB energy, since the leading superpartial forms an APB fault with its movement [13]. Likewise, if a dislocation node belonging to the trailing superpartial lies inside a voxel with a precipitate, the precipitate exerts a positive force of γ per unit length on the dislocation, where γ is the APB energy, since the trailing superpartial repairs an APB fault with its movement [13]. If the dislocation node is in the matrix, no precipitate force is exerted on the dislocation. Constant stresses ranging from 600 – 1000 MPa in steps of 50 MPa, along a single-slip [123] direction, were applied on the dislocation. The minimum stress at which the Frank-Read source continuosly moves through the {111} glide plane and multiplies, was

considered the percolation stress for the source. 36 different random instantiations of the Frank-Read source were considered for the smallest size and 12 different instantiations was considered for the largest size. For the intermediate size, 2 different SEM micrographs were used to obtain precipitate size and spatial positions and, for each micrograph, 12 different random instantiations of the Frank-Read source were simulated.

Figure 2 is a plot of the critical percolation stress as a function of size obtained for the Frank-Read sources for the present 2D dislocation dynamics simulations using a matrix friction stress [15] ~ 250 MPa [10]. Also shown is the experimental 0.2% yield stress data for the same superalloy, multiplied by the Schmidt factor and scaled by the shear modulus, ~ 79 GPa [4]. It is clear that the weakly increasing yield stress with decreasing size as well as the scatter in yield stress at each size observed in the experiment, is approximately reproduced in the simulations. For most cases of simulation, the Frank-Read source bows, interacts with the surface and forms two single-arm sources. Subsequently, the weaker of the two single-arm sources, with one end pinned inside the crystal and the other end on the surface, controls the critical percolation stress for the superdislocation. In some cases, the initial Frank-read source is the critical configuration, where both ends are pinned inside the crystal. Also shown in Fig.2 is the experimental microscopic proportional limit (< 0.001 % flow stress) which is approximately a factor of two below the macroscopic proportional limit, 0.2% flow stress [4]. It is assumed here that the simulated Frank-Read source critical stress data is more representative of the macroscopic proportional limit and that the microscopic proportional limit is most probably caused by a partial movement of a few dislocations on different slip systems. However, verification of this conjecture requires a complete 3D dislocation dynamics

simulation with several interacting Frank-Read sources on different slip systems and has not been performed here.

Figure 3 is a plot of the critical stress obtained for the 36 different instantiations of the Frank-Read source at the 2.75 X 4.125 micron size, versus b/l, where 'l' is the single-arm source length at the critical configuration. If the critical configuration was a Frank-Read source, it's effective single-arm source length was taken to be half the length of the Frank-Read source [16]. A linear fit to the critical stress data gives an equation of the form:

$$\sigma \sim 668 \text{ MPa} + (0.68/S)\mu b/l \qquad (1)$$

where 'S' is the Schmidt factor. In equation (1), 668 MPa is the critical stress at infinite single-arm source length and can be taken to be the precipitation hardening contribution for an infinite material. This value plus the solid solution hardening component of ~ 250 MPa, corresponds closely to the minimum in critical stress observed at larger sizes (see Figure 2). The second term, $(0.68/S)\mu b/l$ is interpreted as the hardening contribution from the single-arm source and corresponds closely to the calculated results for single-arm sources given in reference [16]. However, Figure 3 shows that there is a significant amount of scatter, about the average straight line fit given by equation (1), which is the result of precipitate size and spatial distribution.

Figure 4 is a plot of the critical single-arm source configurations for two different instantiations of the Frank-Read source in the 2.75 X 4.125 μm cell, along with the precipitate configuration. For the two cases, the critical single arm source lengths are almost identical and equal to ~ 1100 nm. However, the critical stress in one case is 900 MPa whereas in the second case, it is much lower and equal to 700 MPa.

Examination of the precipitate configuration at the critical single-arm source positions for the two examples shows that they are significantly different. For the instantitiation having the higher critical stress the single-arm source is almost completely blocked by the precipitate, whereas for the instantiation having the lower critical stress, the single-arm source is only partially blocked by the precipitates. This result suggests that specific precipitate structure at the critical single-arm source positions is also important in determining the critical stress. This additional effect in superalloys can cause the precipitation hardening contribution to increase from the infinite material value, $1/S(\gamma/2b)f$, where f is a fraction less than 1, to a situation where the superdislocation single-arm source is completely blocked by precipitates, $1/S(\gamma/2b)$. Critical single-arm source configurations and sizes for which the statistics of the channels in the precipitate distribution are significantly different from those for an infinite material are expected to show this effect. Therefore, the size effect and scatter in yield stress of superalloys are related to two factors: 1) the strength of single-arm sources and 2) the variation in precipitate structure at the single arm source positions. The stress, $1/S(\gamma/2b)$, plus any solid solution strengthening in the precipitate can be taken to be the limiting stress value, beyond which there will not be any strengthening in micron-sized crystals of superalloys. Such a condition is valid for the assumptions that the stress to nucleate superdislocations at a surface is low and the mobility of freshly nucleated superdislocations controls the yield stress [17]. However, the experimental data [4] does not show any such tendency for a saturation stress value, most likely because the experimental size-effect data does not include small enough sizes of micron-sized crystals of superalloys.

Finally, it has to be noted that the APB energy of the experimental superalloy is unknown and, the solid-solution-hardening contribution assumed in the comparison of simulation to the experimental data is approximate. Also, strain hardening effects from forest dislocations as well as thermally activated processes like cross-slip in the γ matix or γ' precipitate were not considered in the simulations. In light of these considerations, it is suggested that the modified source-truncation mechanism be taken as one possible explanation for the observed weak size effect in initial yield, as well as the scatter in yield stress at each size in experiments of micron-sized crystals of superalloys.

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Figure Captions:

1) Scanning Electron Micrographs of γ' precipitate distribution on {111} glide planes, A) 11 X 16.5, B) 5.5 X 8.25 and C) 2.75 X 4.125 μm in size. The x axis is along [3 -4 1] and the y axis is along [5 2 -7]. The precipitates are in black and the matrix in white. The two insets in A give the 5.5 X 8.25 and 2.75 X 4.125 μm regions of B and C.

2) Critical percolation stress as a function of size obtained for the Frank-Read sources with the present 2D dislocation dynamics simulations plus matrix friction stress ~ 250 Mpa, as well as the experimental 0.2% yield stress data (macroscopic proportional limit) and experimental microscopic proportional limit, for the same superalloy, multiplied by the Schmidt factor and scaled by the shear modulus .

3) Critical stress, σ obtained for 36 different instantiations of the Frank-Read source at the 2.75 X 4.125 micron size, versus b/l, where 'l' is the effective single-arm source length at the critical configuration.

4) Plot of the critical single-arm source configurations for two different instantiations of the Frank-Read source in the 2.75 X 4.125 μm cell, along with the precipitate configuration. The x axis is along [3 -4 1] and the y axis is along [5 2 -7]. The precipitates are in white and the matrix in black. The arrows point to the critical single-arm source configurations.

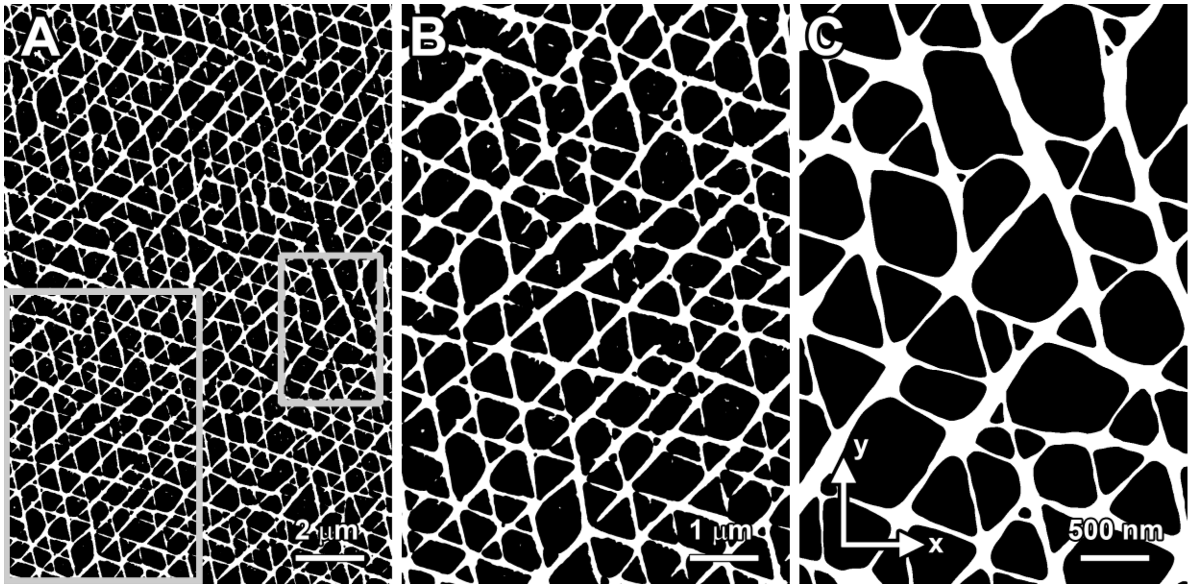

Fig.1:

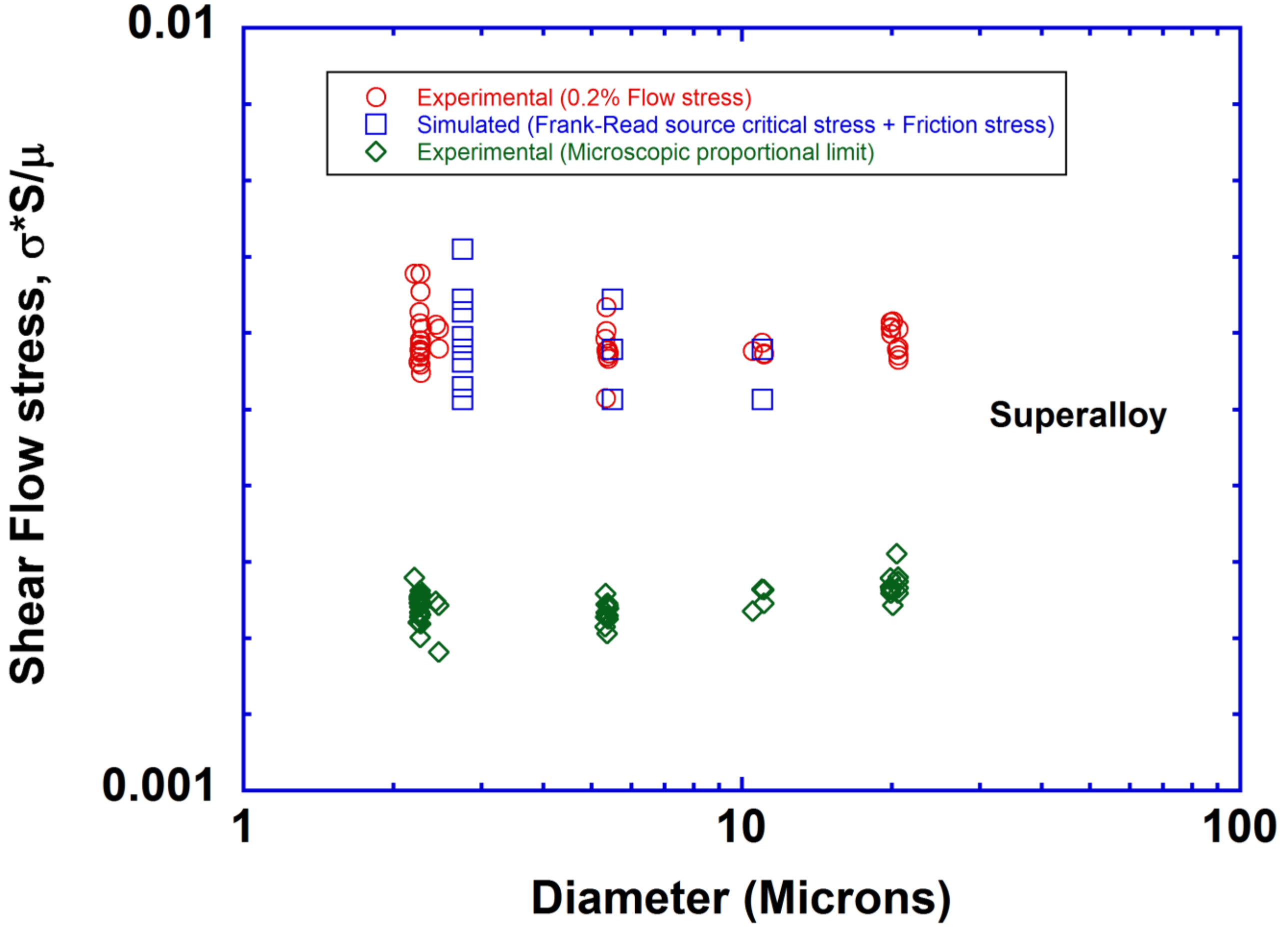
Experimental (0.2% Flow stress)
Simulated (Frank-Read source critical stress + Friction stress)
Experimental (Microscopic proportional limit)
Superalloy
Shear Flow stress, σ*S/μ
0.01
0.001
1
10
100
Diameter (Microns)

Fig.2 :

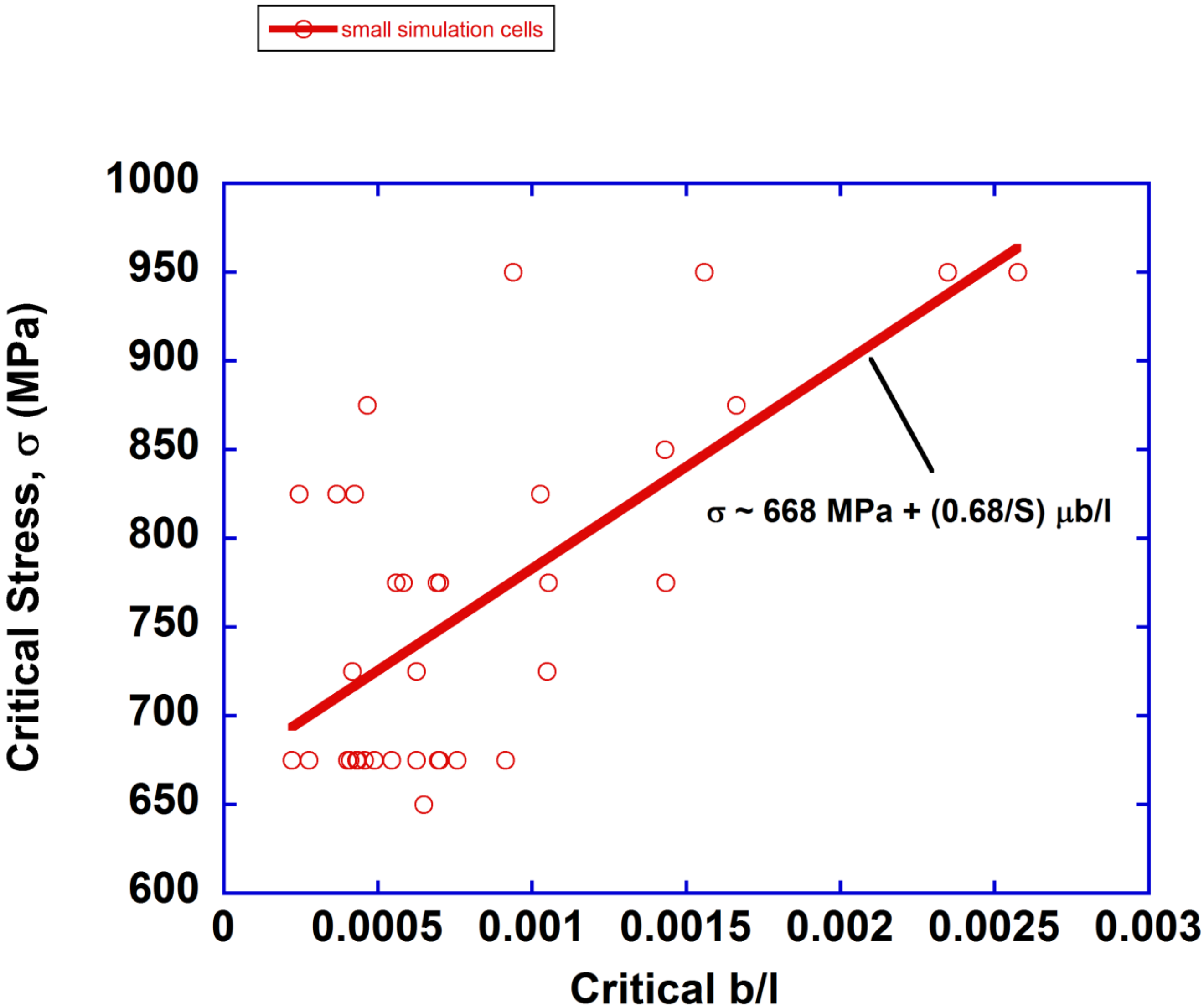
small simulation cells
σ ~ 668 MPa + (0.68/S) μb/l
Critical Stress, σ (MPa)
Critical b/l
1000
950
900
850
800
750
700
650
600
0
0.0005
0.001
0.0015
0.002
0.0025
0.003

Fig. 3:

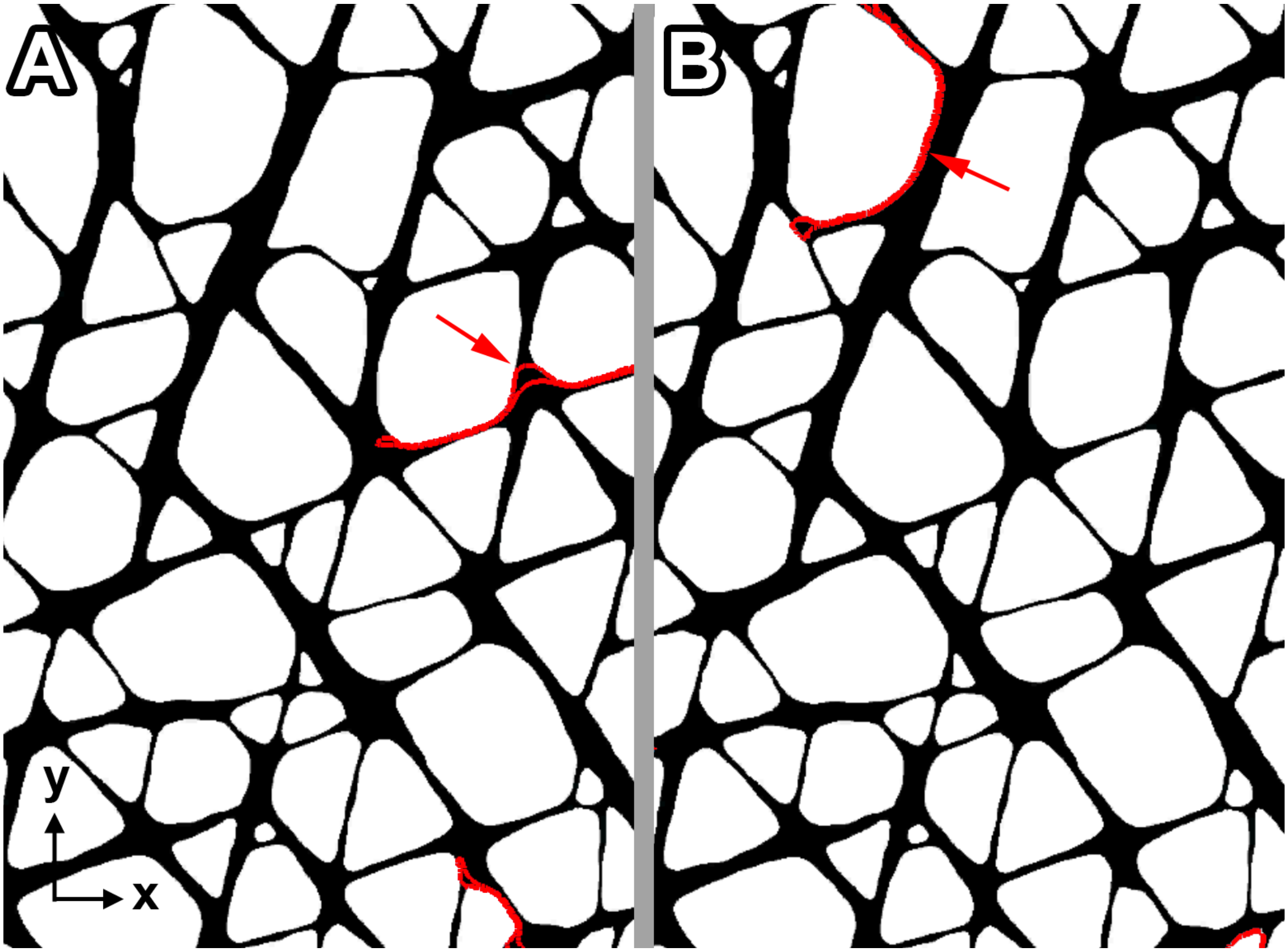

Fig.4: